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1,3-Bis(3,4-dimethoxyphenyl)prop-2-en-1-one

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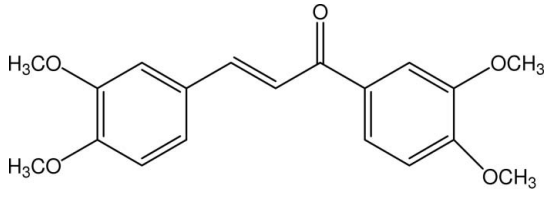
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.002 Å; R factor = 0.054; wR factor = 0.163; data-to-parameter ratio = 22.7.

In the title compound, $C_{19}H_{20}O_5$, the dihedral angle between the benzene rings is 5.92 (6)°. The molecules are linked by two pairs of C—H···O hydrogen bonds into a centrosymmetric dimer of $R_2^1(6)$ ring motif. In addition, the crystal structure is stabilized by C—H···π interactions.

Related literature

For hydrogen-bond motifs, see Bernstein *et al.* (1995). For bond-length data, see Allen *et al.* (1987). For related literature, see Patil *et al.* (2006); Patil, Dharmaprakash *et al.* (2007); Patil, Teh, Fun, Babu *et al.* (2007); Patil, Teh, Fun, Razak *et al.* (2007).



Experimental

Crystal data

$C_{19}H_{20}O_5$
M_r = 328.35
Monoclinic, $P2_1/c$
a = 9.3543 (2) Å
b = 7.9014 (2) Å
c = 24.0405 (6) Å
β = 106.148 (2)°
V = 1706.78 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 297 (2) K
0.55 × 0.42 × 0.34 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.961, T_{max} = 0.970
21071 measured reflections
5021 independent reflections
2222 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.163
S = 1.03
5021 reflections
221 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C1–C6 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O3^{i}	0.93	2.54	3.390 (2)	151
C7—H7···O3^{i}	0.93	2.49	3.357 (2)	155
C17—H17*C*···*Cg*1^{ii}	0.96	2.98	3.865 (2)	154

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $-x+1, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PLATON* (Spek, 2003) and *PARST* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2365).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12a) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Patil, P. S., Dharmaprakash, S. M., Fun, H.-K. & Karthikeyan, M. S. (2006). *J. Cryst. Growth*, **297**, 111–116.
Patil, P. S., Dharmaprakash, S. M., Ramakrishna, K., Fun, H.-K., Sai Santosh Kumar, R. & Narayana Rao, D. (2007). *J. Cryst. Growth*. In the press.
Patil, P. S., Teh, J. B.-J., Fun, H.-K., Babu, H. B. R., Razak, I. A. & Dharmaprakash, S. M. (2007). *Acta Cryst.* E**63**, o1895–o1896.
Patil, P. S., Teh, J. B.-J., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2007). *Acta Cryst.* E**63**, o2122–o2123.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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supplementary materials

Acta Cryst. (2007). E**63**, o2613 [**doi:10.1107/S160053680701865X**]

1,3-Bis(3,4-dimethoxyphenyl)prop-2-en-1-one

J. B.-J. Teh, P. S. Patil, H.-K. Fun, I. A. Razak and S. M. Dharmaprakash

Comment

Many chalcone derivatives display significant second-order nonlinear optical (NLO) properties (Patil *et al.*, 2006; Patil, Dharmaprakash *et al.*, 2007). As part of our ongoing studies in this area (Patil, Teh, Fun, Babu *et al.*, 2007; Patil, Teh, Fun, Razak *et al.*, 2007), we have prepared the title chalcone derivative, (I) (Fig. 1). Crystals of (I) do not exhibit second-order nonlinear

optical properties as they crystallize in a centrosymmetric space group.

Bond lengths and angles in (I) show normal values (Allen *et al.*, 1987) and are comparable with those in related structures (Patil, Teh, Fun, Ramesh Babu *et al.*, 2007; Patil, Teh, Fun, Razak *et al.*, 2007). The enone group (C7–C9/O3) makes dihedral angles of 1.15 (7) and 4.79 (7)°, respectively, with the C1–C6 and C10–C15 benzene rings. The dihedral angle between the benzene rings is 5.92 (6)°. The four methoxy groups are almost coplanar with the attached rings,

as shown by the C16—O1—C2—C1, C17—O2—C3—C4, C18—O4—C12—C11 and C19—O5—C13—C14 torsion angles of -6.4 (3), -2.1 (3), 3.8 (3) and 3.3 (3)°, respectively.

In the crystal structure (Fig. 2), the C5—H5···O3^{i} and C7—H7···O3^{i} intermolecular interactions [Table 1; symmetry code: (i) -x, 2-y, -z] form a pair of bifurcated acceptor bonds, which generate a centrosymmetric dimer of $R^{1}_{2}(6)$ ring motif (Bernstein *et al.*, 1995). The crystal structure is further stabilized by C—H···π interactions (Table 1) involving the C1–C6 benzene ring (centroid Cg1).

Experimental

3,4-Dimethoxybenzaldehyde (0.01 mol) and 3,4-dimethoxyacetophenone (0.01 mol) were stirred in methanol (60 ml) at room temperature. 20% NaOH aqueous solution

(20 ml) was added and the mixture was stirred for 6 h. The resulting precipitate was filtered off, washed with water and dried. The crude product was recrystallized from acetone. Single crystals suitable for X-ray analysis were obtained by slow evaporation of an acetone solution at room temperature.

Refinement

H atoms were positioned geometrically and treated as riding, with C—H = 0.93 or 0.96 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

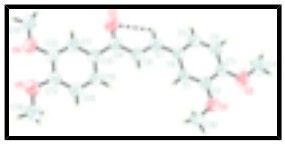

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed line indicates a hydrogen bond.

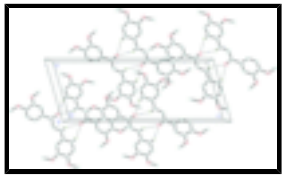

Fig. 2. The crystal packing of (I), viewed down the *b* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in the hydrogen bonds have been omitted for clarity.

1,3-Bis(3,4-dimethoxyphenyl)prop-2-en-1-one

Crystal data

$C_{19}H_{20}O_5$	F_{000} = 696
M_r = 328.35	D_x = 1.278 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3229 reflections
a = 9.3543 (2) Å	θ = 2.3–30.1°
b = 7.9014 (2) Å	μ = 0.09 mm^{-1}
c = 24.0405 (6) Å	T = 297 (2) K
β = 106.148 (2)°	Block, yellow
V = 1706.78 (7) Å^3	0.55 × 0.42 × 0.34 mm
Z = 4	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	5021 independent reflections
Radiation source: fine-focus sealed tube	2222 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 30.1°
T = 297(2) K	θ_{min} = 2.3°
ω scans	h = −13→13
Absorption correction: multi-scan (SADABS; Bruker, 2005)	k = −8→11
T_{min} = 0.961, T_{max} = 0.970	l = −33→33
21071 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 0.0194P]$ where $P = (F_o^2 + 2F_c^2)/3$

$R[F^2 > 2\sigma(F^2)] = 0.054$

$wR(F^2) = 0.163$

$S = 1.03$

5021 reflections

221 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.13$ e Å^{-3}

$\Delta\rho_{min} = -0.15$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.67098 (13)	0.57700 (17)	0.16281 (5)	0.0677 (4)
O2	0.75255 (13)	0.59791 (19)	0.06831 (5)	0.0759 (4)
O3	−0.08215 (15)	1.0025 (2)	0.06712 (5)	0.0941 (5)
O4	−0.38043 (13)	1.09985 (18)	0.20964 (5)	0.0733 (4)
O5	−0.22752 (14)	0.96920 (17)	0.30656 (5)	0.0698 (4)
C1	0.43616 (18)	0.7133 (2)	0.11822 (7)	0.0543 (5)
H1	0.4059	0.7016	0.1517	0.065*
C2	0.57227 (18)	0.6523 (2)	0.11712 (7)	0.0536 (4)
C3	0.61759 (19)	0.6654 (2)	0.06602 (7)	0.0591 (5)
C4	0.5246 (2)	0.7434 (3)	0.01857 (7)	0.0720 (6)
H4	0.5538	0.7533	−0.0152	0.086*
C5	0.3879 (2)	0.8078 (3)	0.02014 (7)	0.0678 (5)
H5	0.3271	0.8611	−0.0124	0.081*
C6	0.34124 (18)	0.7934 (2)	0.06965 (7)	0.0558 (5)
C7	0.19693 (19)	0.8618 (2)	0.07048 (7)	0.0618 (5)
H7	0.1403	0.9114	0.0364	0.074*
C8	0.13802 (19)	0.8609 (2)	0.11453 (7)	0.0618 (5)
H8	0.1914	0.8103	0.1490	0.074*
C9	−0.0071 (2)	0.9355 (2)	0.11174 (7)	0.0610 (5)
C10	−0.06215 (18)	0.9333 (2)	0.16383 (7)	0.0522 (4)
C11	−0.19713 (18)	1.0139 (2)	0.16105 (7)	0.0555 (5)
H11	−0.2515	1.0622	0.1263	0.067*

C12	−0.25045 (18)	1.0230 (2)	0.20840 (7)	0.0535 (4)
C13	−0.16737 (19)	0.9508 (2)	0.26100 (7)	0.0560 (5)
C14	−0.03606 (19)	0.8694 (2)	0.26395 (7)	0.0610 (5)
H14	0.0183	0.8205	0.2986	0.073*
C15	0.01550 (19)	0.8599 (2)	0.21544 (7)	0.0581 (5)
H15	0.1040	0.8031	0.2176	0.070*
C16	0.6347 (2)	0.5778 (3)	0.21637 (7)	0.0736 (6)
H16A	0.7159	0.5310	0.2461	0.110*
H16B	0.5469	0.5110	0.2129	0.110*
H16C	0.6167	0.6919	0.2264	0.110*
C17	0.7989 (2)	0.6041 (3)	0.01652 (8)	0.0914 (7)
H17A	0.8921	0.5461	0.0226	0.137*
H17B	0.8104	0.7200	0.0065	0.137*
H17C	0.7253	0.5505	−0.0144	0.137*
C18	−0.4705 (2)	1.1666 (3)	0.15663 (8)	0.0774 (6)
H18A	−0.5612	1.2104	0.1623	0.116*
H18C	−0.4935	1.0786	0.1280	0.116*
H18B	−0.4179	1.2560	0.1437	0.116*
C19	−0.1418 (3)	0.9055 (3)	0.36133 (8)	0.0897 (7)
H19C	−0.1914	0.9313	0.3903	0.135*
H19A	−0.0452	0.9573	0.3716	0.135*
H19B	−0.1313	0.7851	0.3589	0.135*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0567 (8)	0.0852 (10)	0.0633 (7)	0.0140 (7)	0.0199 (6)	0.0091 (7)
O2	0.0597 (8)	0.1047 (11)	0.0700 (8)	0.0131 (7)	0.0292 (6)	−0.0088 (7)
O3	0.0822 (10)	0.1380 (15)	0.0661 (9)	0.0465 (10)	0.0273 (7)	0.0263 (9)
O4	0.0603 (8)	0.0915 (11)	0.0706 (8)	0.0226 (7)	0.0223 (6)	0.0034 (7)
O5	0.0727 (8)	0.0810 (10)	0.0593 (7)	0.0073 (7)	0.0245 (6)	−0.0009 (6)
C1	0.0559 (11)	0.0594 (12)	0.0521 (9)	0.0004 (9)	0.0224 (8)	−0.0002 (8)
C2	0.0500 (10)	0.0582 (12)	0.0521 (9)	−0.0001 (9)	0.0133 (8)	−0.0010 (8)
C3	0.0525 (11)	0.0672 (13)	0.0607 (10)	0.0012 (9)	0.0206 (8)	−0.0068 (9)
C4	0.0727 (13)	0.0936 (16)	0.0565 (11)	0.0063 (12)	0.0291 (10)	0.0025 (10)
C5	0.0657 (12)	0.0835 (15)	0.0558 (10)	0.0111 (11)	0.0194 (9)	0.0103 (9)
C6	0.0536 (10)	0.0609 (12)	0.0549 (10)	0.0032 (9)	0.0182 (8)	0.0014 (9)
C7	0.0578 (11)	0.0684 (13)	0.0583 (10)	0.0073 (9)	0.0147 (8)	0.0053 (9)
C8	0.0587 (11)	0.0703 (13)	0.0566 (10)	0.0139 (10)	0.0164 (8)	0.0030 (9)
C9	0.0583 (11)	0.0667 (13)	0.0570 (10)	0.0100 (10)	0.0147 (9)	0.0027 (9)
C10	0.0517 (10)	0.0500 (11)	0.0546 (9)	0.0030 (8)	0.0140 (8)	−0.0027 (8)
C11	0.0525 (10)	0.0571 (12)	0.0529 (9)	0.0055 (9)	0.0082 (8)	−0.0019 (8)
C12	0.0474 (10)	0.0536 (12)	0.0589 (10)	0.0023 (8)	0.0138 (8)	−0.0055 (8)
C13	0.0589 (11)	0.0527 (12)	0.0571 (10)	−0.0039 (9)	0.0173 (8)	−0.0066 (8)
C14	0.0573 (11)	0.0661 (13)	0.0574 (10)	0.0093 (10)	0.0123 (8)	0.0083 (9)
C15	0.0539 (10)	0.0551 (12)	0.0644 (11)	0.0073 (9)	0.0149 (8)	0.0019 (9)
C16	0.0699 (13)	0.0931 (16)	0.0571 (11)	0.0074 (11)	0.0165 (9)	0.0116 (10)
C17	0.0727 (14)	0.137 (2)	0.0752 (13)	0.0074 (14)	0.0383 (11)	−0.0219 (13)

C18	0.0624 (12)	0.0841 (16)	0.0814 (13)	0.0231 (11)	0.0128 (10)	0.0030 (11)
C19	0.1086 (17)	0.1071 (19)	0.0558 (11)	0.0154 (15)	0.0268 (11)	0.0106 (11)

Geometric parameters (Å, °)

O1—C2	1.3599 (19)	C9—C10	1.480 (2)
O1—C16	1.4200 (19)	C10—C15	1.379 (2)
O2—C3	1.357 (2)	C10—C11	1.399 (2)
O2—C17	1.428 (2)	C11—C12	1.366 (2)
O3—C9	1.2268 (19)	C11—H11	0.93
O4—C12	1.3667 (19)	C12—C13	1.408 (2)
O4—C18	1.420 (2)	C13—C14	1.371 (2)
O5—C13	1.3712 (18)	C14—C15	1.382 (2)
O5—C19	1.429 (2)	C14—H14	0.93
C1—C2	1.368 (2)	C15—H15	0.93
C1—C6	1.405 (2)	C16—H16A	0.96
C1—H1	0.93	C16—H16B	0.96
C2—C3	1.411 (2)	C16—H16C	0.96
C3—C4	1.373 (2)	C17—H17A	0.96
C4—C5	1.386 (2)	C17—H17B	0.96
C4—H4	0.93	C17—H17C	0.96
C5—C6	1.382 (2)	C18—H18A	0.96
C5—H5	0.93	C18—H18C	0.96
C6—C7	1.460 (2)	C18—H18B	0.96
C7—C8	1.323 (2)	C19—H19C	0.96
C7—H7	0.93	C19—H19A	0.96
C8—C9	1.465 (2)	C19—H19B	0.96
C8—H8	0.93		
C2—O1—C16	116.78 (13)	C11—C12—O4	125.09 (15)
C3—O2—C17	117.08 (15)	C11—C12—C13	119.27 (15)
C12—O4—C18	117.07 (13)	O4—C12—C13	115.63 (14)
C13—O5—C19	116.69 (14)	C14—C13—O5	124.69 (15)
C2—C1—C6	121.24 (14)	C14—C13—C12	119.97 (15)
C2—C1—H1	119.4	O5—C13—C12	115.34 (15)
C6—C1—H1	119.4	C13—C14—C15	119.98 (16)
O1—C2—C1	124.40 (14)	C13—C14—H14	120.0
O1—C2—C3	115.76 (15)	C15—C14—H14	120.0
C1—C2—C3	119.84 (16)	C10—C15—C14	121.07 (16)
O2—C3—C4	125.27 (15)	C10—C15—H15	119.5
O2—C3—C2	115.93 (16)	C14—C15—H15	119.5
C4—C3—C2	118.81 (16)	O1—C16—H16A	109.5
C3—C4—C5	121.21 (16)	O1—C16—H16B	109.5
C3—C4—H4	119.4	H16A—C16—H16B	109.5
C5—C4—H4	119.4	O1—C16—H16C	109.5
C6—C5—C4	120.52 (17)	H16A—C16—H16C	109.5
C6—C5—H5	119.7	H16B—C16—H16C	109.5
C4—C5—H5	119.7	O2—C17—H17A	109.5
C5—C6—C1	118.35 (15)	O2—C17—H17B	109.5
C5—C6—C7	119.75 (16)	H17A—C17—H17B	109.5

C1—C6—C7	121.90 (14)	O2—C17—H17C	109.5
C8—C7—C6	127.00 (16)	H17A—C17—H17C	109.5
C8—C7—H7	116.5	H17B—C17—H17C	109.5
C6—C7—H7	116.5	O4—C18—H18A	109.5
C7—C8—C9	123.26 (17)	O4—C18—H18C	109.5
C7—C8—H8	118.4	H18A—C18—H18C	109.5
C9—C8—H8	118.4	O4—C18—H18B	109.5
O3—C9—C8	120.76 (16)	H18A—C18—H18B	109.5
O3—C9—C10	119.71 (16)	H18C—C18—H18B	109.5
C8—C9—C10	119.51 (15)	O5—C19—H19C	109.5
C15—C10—C11	118.48 (15)	O5—C19—H19A	109.5
C15—C10—C9	123.09 (15)	H19C—C19—H19A	109.5
C11—C10—C9	118.41 (15)	O5—C19—H19B	109.5
C12—C11—C10	121.20 (15)	H19C—C19—H19B	109.5
C12—C11—H11	119.4	H19A—C19—H19B	109.5
C10—C11—H11	119.4		
C16—O1—C2—C1	−6.4 (3)	O3—C9—C10—C15	179.77 (18)
C16—O1—C2—C3	173.75 (15)	C8—C9—C10—C15	−1.7 (3)
C6—C1—C2—O1	178.49 (16)	O3—C9—C10—C11	−2.2 (3)
C6—C1—C2—C3	−1.7 (3)	C8—C9—C10—C11	176.37 (16)
C17—O2—C3—C4	−2.1 (3)	C15—C10—C11—C12	1.1 (3)
C17—O2—C3—C2	177.85 (17)	C9—C10—C11—C12	−176.99 (16)
O1—C2—C3—O2	1.4 (2)	C10—C11—C12—O4	179.64 (16)
C1—C2—C3—O2	−178.40 (16)	C10—C11—C12—C13	0.4 (3)
O1—C2—C3—C4	−178.63 (17)	C18—O4—C12—C11	3.8 (3)
C1—C2—C3—C4	1.5 (3)	C18—O4—C12—C13	−176.98 (16)
O2—C3—C4—C5	179.54 (18)	C19—O5—C13—C14	3.3 (3)
C2—C3—C4—C5	−0.4 (3)	C19—O5—C13—C12	−176.65 (17)
C3—C4—C5—C6	−0.6 (3)	C11—C12—C13—C14	−1.4 (3)
C4—C5—C6—C1	0.5 (3)	O4—C12—C13—C14	179.34 (16)
C4—C5—C6—C7	−179.96 (18)	C11—C12—C13—O5	178.57 (15)
C2—C1—C6—C5	0.7 (3)	O4—C12—C13—O5	−0.7 (2)
C2—C1—C6—C7	−178.87 (16)	O5—C13—C14—C15	−179.22 (16)
C5—C6—C7—C8	−178.66 (19)	C12—C13—C14—C15	0.7 (3)
C1—C6—C7—C8	0.9 (3)	C11—C10—C15—C14	−1.8 (3)
C6—C7—C8—C9	178.91 (18)	C9—C10—C15—C14	176.23 (16)
C7—C8—C9—O3	0.5 (3)	C13—C14—C15—C10	0.9 (3)
C7—C8—C9—C10	−178.07 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O3^{i}	0.93	2.54	3.390 (2)	151
C7—H7···O3^{i}	0.93	2.49	3.357 (2)	155
C17—H17C···Cg1^{ii}	0.96	2.98	3.865 (2)	154

Symmetry codes: (i) −*x*, −*y*+2, −*z*; (ii) −*x*+1, −*y*+1, −*z*.

Fig. 1

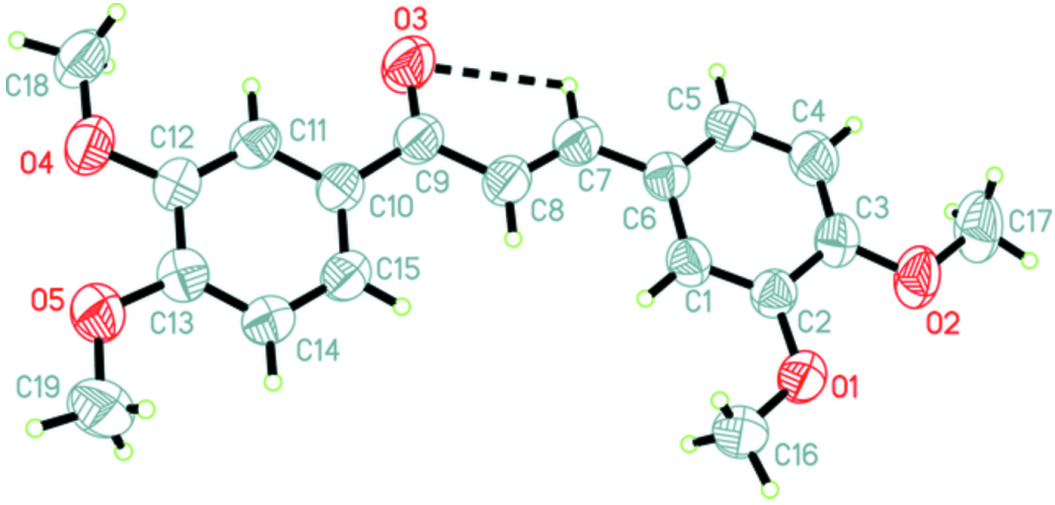
O3
C18
C12
C11
C5
C4
O4
C9
C7
C10
C8
C6
C3
C17
C15
O5
C13
C1
O2
C2
C14
O1
C19
C16

Fig. 2